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### Lewis Research Center



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# Carbon Monoxide Oxidation Rates Computed for Automobile Thermal Reactor Conditions

Carbon monoxide oxidation rates have been computed by integrating differential equations for a system of 29 reversible chemical reactions. At temperatures above 1030°K (1394°F), oxidation is rapid and is complete in one-fourth of the residence time in thermal reactors for exhaust manifolds.

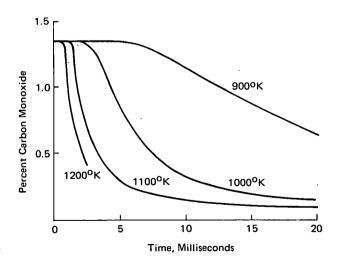
The reactors are noncatalytic replacements for conventional exhaust manifolds and are a system for reducing carbon monoxide and hydrocarbons in automobile exhausts. Secondary air is injected at the cylinder exhaust ports and reacts with pollutants in a well-insulated container which replaces the usual exhaust manifold. The thermal reactor provides volume both for mixing the added air with the exhaust gas and for the subsequent reaction.

Concentrations of the various chemical species as a function of time were determined by summing the extent of reaction of a large number of simultaneous and competing chemical reactions. In these, the individual rates are dependent on concentration and temperature; temperature, in turn, depends on changes in composition. Solution for temperature and composition requires the integration of a set of first order, nonlinear differential equations. The system was assumed to be adiabatic and to obey the ideal gas law. Carbon monoxide and hydrogen are the major combustibles in the untreated exhaust gas and may amount to several percent by volume. Hydrocarbon concentrations are considerably smaller amounting to several hundred parts per million.

Carbon monoxide oxidation rates for various initial temperatures are shown in the figure. The residence time in a typical thermal reactor is about 20 milliseconds; whereas, at temperatures somewhat above 1100° K (1520°F), oxidation is substantially complete in 5 milliseconds. Thus the reactor volume must serve principally to mix exhaust and added air rather than to provide time for reaction. There is a temperature limit at about

1030°K (1394°F) above which reaction is rapid. Any further increases in temperature do not speed up the reaction. Since reaction is slower at lower temperatures, the exhaust manifold reactors do not perform as well.

Calculations were carried out for exhaust gas compositions corresponding to idle and cruise conditions with dilution air added to bring the compositions to stoichiometric condition and to a leaner air-fuel ratio of 17:1. Mixtures diluted to stoichiometric conditions had residual carbon monoxide concentrations of 0.2 to 0.5 percent when the initial temperature was 1100°K(1520°F) or above. Mixtures diluted to an air-fuel ratio of 17:1 had carbon monoxide concentrations of 0.05 percent in 5 milliseconds or less when initial temperatures were 1100°K(1520°F) or above. Thus, excess air definitely promotes the final cleanup of the last traces of carbon monoxide.



(continued overleaf)

#### Notes:

- 1. With the rate limiting process identified, a more rational design of the thermal reactor should be possible.
- 2. The following documentation may be obtained from:
  National Technical Information Service
  Springfield, Virginia 22151
  Single document price \$3.00
  (or microfiche \$0.95)

Reference: NASA TN-D-7024 (N71-12066), Carbon Monoxide Oxidation Rates Computed for Automobile Exhaust Manifold Reactor Conditions. 3. Technical questions may be directed to:

Technology Utilization Officer Lewis Research Center 21000 Brookpark Road Cleveland, Ohio 44135 Reference: TSP72-10137

### Patent status:

No patent action is contemplated by NASA.

Source: R. S. Brokaw and D. A. Bittker of Lewis Research Center (LEW-11638)